Reduced–Basis Output Bound Methods for Parametrized Partial Differential Equations

Christophe Prud'Homme, D.V Rovas, K. Veroy, L. Machiels, Yvon Maday, Anthony T. Patera, Gabriel Turinici

Reduced-Basis Output Bound Methods for Parametrized Partial Differential Equations

C. Prud'homme, D.V. Rovas, K. Veroy, L. Machiels, Y. Maday, A.T. Patera, and G. Turinici

Abstract— **We present a technique for the *rapid* and *reliable* prediction of linear–functional outputs of elliptic (and parabolic) partial differential equations with affine parameter dependence. The essential components are (*i*) (provably) rapidly convergent global reduced–basis approximations — Galerkin projection onto a space W_N spanned by solutions of the governing partial differential equation at N selected points in parameter space; (*ii*) *a posteriori* error estimation — relaxations of the error–residual equation that provide inexpensive yet sharp and rigorous bounds for the error in the outputs of interest; and (*iii*) off–line/on–line computational procedures — methods which decouple the generation and projection stages of the approximation process. The operation count for the on–line stage — in which, given a new parameter value, we calculate the output of interest and associated error bound — depends only on N (typically very small) and the parametric complexity of the problem; the method is thus ideally suited for the repeated and rapid evaluations required in the context of parameter estimation, design, optimization, and real–time control.**

Keywords— **reduced–basis, *a posteriori* error estimation, output bounds, partial differential equations**

I. Introduction

The optimization, control, and characterization of an engineering component or system requires the prediction of certain "quantities of interest," or performance metrics, which we shall denote *outputs* — for example deflections, maximum stresses, maximum temperatures, heat transfer rates, flowrates, or lift and drags. These outputs are typically expressed as functionals of field variables associated with a parametrized partial differential equation which describes the physical behavior of the component or system. The parameters, which we shall denote *inputs*, serve to identify a particular "configuration" of the component: these inputs may represent design or decision variables, such as geometry — for example, in optimization studies; control variables, such as actuator power — for example, in real–time applications; or characterization variables, such as physical properties — for example, in inverse problems. We thus arrive at an implicit *input–output* relationship, evaluation of which demands solution of the underlying partial differential equation.

Our goal is the development of computational methods that permit *rapid* and *reliable* evaluation of this partial-differential-equation-induced input-output relationship *in the limit of many queries* — that is, in the design, optimization, control, and characterization contexts. The "many query" limit has certainly received considerable attention: from "fast loads" or multiple right-hand side notions (e.g., [1], [2]) to matrix perturbation theories (e.g., [3], [4]) to continuation methods (e.g., [5], [6]). Our particular approach is based upon the reduced–basis method, first introduced in the late 1970s for nonlinear structural analysis [7], [8], and subsequently developed more broadly in the 1980s and 1990s [9], [10], [11], [12], [13]. The reduced–basis method recognizes that the field variable is not, in fact, some arbitrary member of the infinite-dimensional space associated with the partial differential equation; rather, it resides, or "evolves," on a much lower–dimensional manifold induced by the parametric dependence.

The reduced–basis approach as earlier articulated is local in parameter space in both practice and theory. To wit, Lagrangian or Taylor approximation spaces for the low–dimensional manifold are typically defined relative to a particular parameter point; and the associated *a priori* convergence theory relies on asymptotic arguments in sufficiently small neighborhoods [10]. As a result, the computational improvements — relative to conventional (say) finite element approximation — are quite modest [12]. Our work differs from these earlier efforts in several important ways: first, we develop (in some cases, provably) *global* approximation spaces; second, we introduce rigorous *a posteriori error estimators*; and third, we exploit affine parameter dependence and associated *off–line/on–line* computational decompositions (see [14] for an earlier application of this strategy within the reduced–basis context). These three ingredients allow us — for a restricted but important class of problems — to reliably decouple the generation and projection stages of reduced–basis approximation, thereby effecting computational economies of several orders of magnitude.

In this brief paper we describe our approach for the particularly simple case of coercive symmetric operators and "compliant" outputs. In Section I we introduce an abstract problem formulation and illustrative instantiation; in Section II we describe our reduced–basis approximation; and in Section III we present the *a posteriori* error estimation procedure. Extension of the method to noncompliant outputs, nonsymmetric and noncoercive operators, eigenvalue problems, and parabolic equations may be found in [15], [16], [17], [18], [19]. See also [20], [18] for a description of the network system architecture in which our numerical objects reside.

C. Prud'homme, D.V. Rovas, K. Veroy, L. Machiels, and A.T. Patera are with the Massachusetts Institute of Technology, Department of Mechanical Engineering, Bldg. 3-264, Cambridge, MA 02139-4307 USA

Y. Maday is with the Analyse numérique, Université Paris VI, 4, place Jussieu, 75252 Paris cedex 05, France.

G. Turinici is with the ASCI, UPR 9029, bâtiment 506, Université Paris-Sud, 91405 Orsay cedex, France

II. Problem Statement

A. Abstract Formulation

We consider a suitably regular domain $\Omega \subset \mathbb{R}^d$, $d = 1$, 2, or 3, and associated function space $X \subset H^1(\Omega)$, where $H^1(\Omega) = \{v \in L^2(\Omega),\ \nabla v \in (L^2(\Omega))^d\}$, and $L^2(\Omega)$ is the space of square integrable functions over Ω. The inner product and norm associated with X are given by $(\,\cdot\,,\,\cdot\,)_X$ and $\|\cdot\|_X = (\,\cdot\,,\,\cdot\,)^{1/2}$, respectively. We also define a parameter set $\mathcal{D} \in \mathbb{R}^{\mathcal{P}}$, a particular point in which will be denoted μ. Note that Ω does *not* depend on the parameter.

We then introduce a "bilinear" form a: $X \times X \times \mathcal{D} \to \mathbb{R}$, and linear forms f: $X \to \mathbb{R}$, ℓ: $X \to \mathbb{R}$. We shall assume that a is continuous, $a(w, v; \mu) \le \gamma(\mu)\ \|w\|_X\ \|v\|_X \le \gamma_0\ \|w\|_X\ \|v\|_X$, $\forall \mu \in \mathcal{D}$; that a is coercive,

$$0 < \alpha_0 \le\ \alpha(\mu) = \inf_{w \in X} \frac{a(w, w; \mu)}{\|w\|_X^2}, \tag{1}$$

$\forall\ \mu \in \mathcal{D}$; and that a is symmetric, $a(w, v; \mu) = a(v, w; \mu)$, $\forall\ w, v \in X$, $\forall\ \mu \in \mathcal{D}$. We also require that our linear forms f and ℓ be bounded; and for simplicity, we assume a "compliant" output, $\ell(v) = f(v)$, $\forall\ v \in X$.

We shall also make certain assumptions on the parametric dependence of a, f, and ℓ. In particular, we shall suppose that, for some finite (preferably small) integer Q, a may be expressed as

$$a(w, v; \mu)\ =\ \sum_{q=1}^{Q} \sigma^q(\mu)\ a^q(w, v), \tag{2}$$

$\forall\ w, v \in X$, $\forall\ \mu \in \mathcal{D}$, for some σ^q: $\mathcal{D} \to \mathbb{R}$ and a^q: $X \times X \to \mathbb{R}$, $q = 1, \ldots, Q$. This "separability," or "affine," assumption on the parameter dependence is crucial to computational efficiency; however, certain relaxations are possible [18], [21]. For simplicity of exposition, we assume that f and ℓ do not depend on μ; in actual practice, affine dependence is readily admitted.

Our abstract problem statement is then: for any $\mu \in \mathcal{D}$, find $u(\mu) \in X$ such that

$$a(u(\mu), v; \mu)\ =\ f(v), \quad \forall\ v \in X; \tag{3}$$

and $s(\mu) \in \mathbb{R}$ given by

$$s(\mu) = f(u(\mu)). \tag{4}$$

In the language of the introduction, a is our partial differential equation (in weak form), μ is our parameter, $u(\mu)$ is our field variable, and $s(\mu)$ is our output.

B. A Particular Instantiation: Thermal Fin

In this example we consider the two- and three-dimensional thermal fins shown in Figure 1; these examples may be (interactively) accessed on our Web site[1]. The fins consist of a vertical central "post" of conductivity $\tilde{k}_0$ and four horizontal "subfins" of conductivity $\tilde{k}^i$, $i = 1, \ldots, 4$; the fins conduct heat from a prescribed uniform flux source, $\tilde{q}''$, at the root, $\tilde{\Gamma}_{\text{root}}$, through the post and large-surface-area subfins to the surrounding flowing air; the latter is characterized by a sink temperature $\tilde{u}_0$, and prescribed heat transfer coefficient $\tilde{h}$. The physical model is simple conduction: the temperature field in the fin, $\tilde{u}$, satisfies

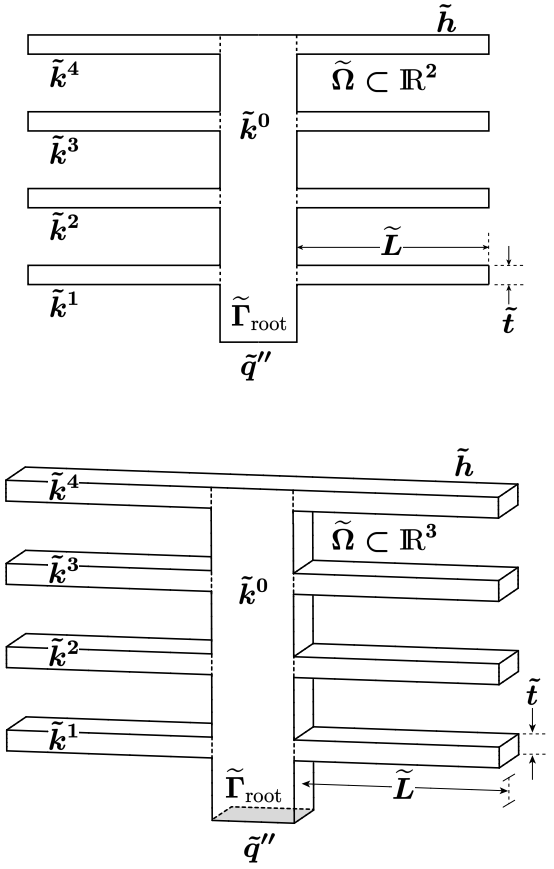

Fig. 1. Two- and Three-Dimensional Thermal Fins.

$$\sum_{i=0}^{4} \int_{\tilde{\Omega}_i} \tilde{k}^i\ \tilde{\nabla}\tilde{u} \cdot \tilde{\nabla}\tilde{v}\ +\ \int_{\partial\tilde{\Omega} \setminus \tilde{\Gamma}_{\text{root}}} \tilde{h}\ (\tilde{u} - \tilde{u}_0)\ \tilde{v}$$

$$= \int_{\tilde{\Gamma}_{\text{root}}} \tilde{q}''\ \tilde{v}, \quad \forall\ \tilde{v} \in \tilde{X} \equiv H^1(\tilde{\Omega}), \tag{5}$$

where $\tilde{\Omega}_i$ is that part of the domain with conductivity $\tilde{k}^i$, and $\partial\tilde{\Omega}$ denotes the boundary of $\tilde{\Omega}$.

We now (i) nondimensionalize the weak equations (5), and (ii) apply a continuous piecewise-affine transformation to map $\tilde{\Omega}$ to a fixed reference domain Ω [16]. The abstract problem statement (3) is then recovered [22] for $\mu = \{k^1,\ k^2,\ k^3,\ k^4,\ \text{Bi},\ L,\ t\}$, $\mathcal{D} = [0.1, 10.0]^4 \times [0.01, 1.0] \times [2.0, 3.0] \times [0.1 \times 0.5]$, and $P = 7$; here $k^1, \ldots, k^4$ are the thermal conductivities of the "subfins" (see Figure 1) relative to the thermal conductivity of the fin base; Bi is a nondimensional form of the heat transfer coefficient;

[1] FIN2D: http://augustine.mit.edu/fin2d/fin2d.pdf and FIN3D: http://augustine.mit.edu/fin3d_1/fin3d_1.pdf

and, L, t are the length and thickness of each of the "subfins" relative to the length of the fin root $\tilde{\Gamma}_{\text{root}}$. It is readily verified that a is continuous, coercive, and symmetric; and that the "affine" assumption (2) obtains for $Q = 16$ (two-dimensional case) and $Q = 25$ (three-dimensional case). Note that the geometric variations are reflected, via the mapping, in the $\sigma^q(\mu)$.

For our output of interest, $s(\mu)$, we consider the average temperature of the root of the fin nondimensionalized relative to $\tilde{q}''$, $\tilde{k}^0$, and the length of the fin root. This output is calculated as $s(\mu) = f(u(\mu))$, where $f(v) = \int_{\Gamma_{\text{root}}} v$.

III. Reduced–Basis Approach

A. Reduced–Basis Approximation

We first introduce a sample in parameter space, $S_N = \{\mu_1, \ldots, \mu_N\}$, where $\mu_i \in \mathcal{D}$, $i = 1, \ldots, N$; see Section III.B for a brief discussion of point distribution. We then define our Lagrangian [12] reduced–basis approximation space as $W_N = \text{span}\ \{\zeta_n \equiv u(\mu_n),\ n = 1, \ldots, N\}$, where $u(\mu_n) \in X$ is the solution to (3) for $\mu = \mu_n$. In actual practice, $u(\mu_n)$ is replaced by a finite element approximation on a suitably fine truth mesh; we shall discuss the associated computational implications in Section III.C. Our reduced–basis approximation is then: for any $\mu \in \mathcal{D}$, find $u_N(\mu) \in W_N$ such that

$$a(u_N(\mu), v; \mu) \ = \ f(v), \quad \forall\ v \in W_N; \tag{6}$$

we then evaluate $s_N(\mu) = f(u_N(\mu))$.

B. A Priori Convergence Theory

B.1 Optimality

We consider here the convergence rate of $u_N(\mu) \rightarrow u(\mu)$ and $s_N(\mu) \rightarrow s(\mu)$ as $N \rightarrow \infty$. To begin, it is standard to demonstrate optimality of $u_N(\mu)$ in the sense that

$$\|u(\mu) - u_N(\mu)\|_X \leq \sqrt{\frac{\gamma(\mu)}{\alpha(\mu)}} \inf_{w_N \in W_N} \|u(\mu) - w_N\|_X \ . \tag{7}$$

(We note that, in the coercive case, stability of our ("conforming") discrete approximation is not an issue; the non-coercive case is decidedly more delicate [17].) Furthermore, for our compliance output,

$$\begin{aligned} s(\mu) &= s_N(\mu) + \ell(u - u_N) \\ &= s_N(\mu) + a(u, u - u_N; \mu) \\ &= s_N(\mu) + a(u - u_N, u - u_N; \mu) \end{aligned} \tag{8}$$

from symmetry and Galerkin orthogonality. It follows that $s(\mu) - s_N(\mu)$ converges as the square of the error in the best approximation and, from coercivity, that $s_N(\mu)$ is a lower bound for $s(\mu)$.

B.2 Best Approximation

It now remains to bound the dependence of the error in the best approximation as a function of N. At present, the theory is restricted to the case in which $P = 1$, $\mathcal{D} = [0, \mu_{\max}]$, and

$$a(w, v; \mu) = a_0(w, v) + \mu a_1(w, v), \tag{9}$$

where a_0 is continuous, coercive, and symmetric, and a_1 is continuous, positive semi-definite ($a_1(w, w) \geq 0, \forall\, w \in X$), and symmetric. This model problem (9) is rather broadly relevant, for example to variable orthotropic conductivity, variable rectilinear geometry, variable piecewise-constant conductivity, and variable Robin boundary conditions.

We now suppose that the μ_n, $n = 1, \ldots, N$, are logarithmically distributed in the sense that

$$\ln\left(\mu_n + \overline{\lambda}^{-1}\right) = \ln \overline{\lambda}^{-1} + \frac{n-1}{N-1} \ln\left(\overline{\lambda}\, \mu_{\max} + 1\right), \tag{10}$$

for $n = 1, \ldots, N$, where $\overline{\lambda}$ is an upper bound for the maximum eigenvalue of a_1 relative to a_0. (Note $\overline{\lambda}$ is perforce bounded thanks to our assumptions of continuity and coercivity; the possibility of a continuous spectrum does not, in practice, pose any problems.) We can then prove [23] that, for $N > N_{\text{crit}} \equiv 1 + e \ln(\overline{\lambda}\, \mu_{\max} + 1)$,

$$\begin{aligned} &\inf_{w_N \in W_N} \|u(\mu) - w_N(\mu)\|_X \\ &\qquad \leq (1 + \mu_{\max}\, \overline{\lambda})\, \|u(0)\|_X\ \exp\left\{\frac{-(N-1)}{(N_{\text{crit}} - 1}\right\}, \end{aligned} \tag{11}$$

$\forall\, \mu \in \mathcal{D}$. We observe exponential convergence, uniformly (globally) for all μ in $\mathcal{D}$, with only very weak (logarithmic) dependence on the range of the parameter ($\mu_{\max}$). (Note the constants in (11) are for the particular case $(\cdot, \cdot)_X \equiv a_0(\cdot, \cdot)$.)

The proof exploits a parameter–space (non-polynomial) interpolant as a surrogate for the Galerkin approximation. As a result, the bound is not "sharp": we observe many cases in which the Galerkin projection is considerably better than the associated interpolant; optimality (7) may choose to "illuminate" only certain points μ_n, automatically selecting a best "sub–approximation" amongst all possibilities. We thus see why reduced–basis *state-space* approximation of $s(\mu)$ via $u(\mu)$ is preferred to simple *parameter-space* interpolation of $s(\mu)$ ("connecting the dots") via $(\mu_n, s(\mu_n))$ pairs. Nevertheless, the logarithmic point distribution (10) suggested by our interpolant–based argument is *not* simply an artifact of the proof: the logarithmic distribution performs considerably (and in many cases, provably) better than other obvious candidates [24], in particular for large ranges of the parameter.

The result (11) is certainly tied to the particular form (9) and associated regularity of $u(\mu)$. However, we do observe similar exponental behavior for more general operators; and, most importantly, the exponential convergence rate degrades only very slowly with increasing parameter dimension, P. We present in Table I the error $|s(\mu) - s_N(\mu)|/s(\mu)$ as a function of N, at a particular representative point μ in $\mathcal{D}$, for the two-dimensional thermal fin problem ($P = 7$) of Section II.B. Since tensor-product grids are prohibitively profligate as P increases, the μ_n

N	$\lvert s(\mu) - s_N(\mu)\rvert / s(\mu)$	$\Delta_N(\mu)/s(\mu)$	$\eta_N(\mu)$
10	1.29×10^{-2}	8.60×10^{-2}	2.85
20	1.29×10^{-3}	9.36×10^{-3}	2.76
30	5.37×10^{-4}	4.25×10^{-3}	2.68
40	8.00×10^{-5}	5.30×10^{-4}	2.86
50	3.97×10^{-5}	2.97×10^{-4}	2.72
60	1.34×10^{-5}	1.27×10^{-4}	2.54
70	8.10×10^{-6}	7.72×10^{-5}	2.53
80	2.56×10^{-6}	2.24×10^{-5}	2.59

TABLE I

ERROR, ERROR BOUND, AND EFFECTIVITY AS A FUNCTION OF N, AT A PARTICULAR REPRESENTATIVE POINT $\mu \in \mathcal{D}$, FOR THE TWO-DIMENSIONAL THERMAL FIN PROBLEM.

are chosen "log-randomly" over $\mathcal{D}$: we sample from a multivariate uniform probability density on $\log(\mu)$. We observe that the error is remarkably small even for very small N; and that very rapid convergence obtains as $N \to \infty$. We do not yet have any theory for $P > 1$. But certainly the Galerkin optimality plays a central role, automatically selecting "appropriate" scattered-data subsets of S_N and associated "good" weights so as to mitigate the curse of dimensionality as P increases; and the logarithmic point distribution is also important, yielding significantly more accurate results [20].

C. Computational Procedure

The theoretical and empirical results of Sections III.A and III.B suggest that N may, indeed, be chosen very small. We now develop off–line/on–line computational procedures that exploit this dimension reduction.

We first express $u_N(\mu)$ as

$$u_N(\mu) = \sum_{j=1}^{N} u_{N\,j}(\mu)\, \zeta_j = (\underline{u}_N(\mu))^T\, \underline{\zeta}, \qquad (12)$$

where $\underline{u}_N(\mu) \in \mathbb{R}^N$; we then choose for test functions $v = \zeta_i$, $i = 1, \ldots, N$. Inserting these representations into (6) yields the desired algebraic equations for $\underline{u}_N(\mu) \in \mathbb{R}^N$,

$$\underline{A}_N(\mu)\, \underline{u}_N(\mu) \;=\; \underline{F}_N \qquad (13)$$

in terms of which the output can then be evaluated as $s_N(\mu) = \underline{F}_N^T\, \underline{u}_N(\mu)$. Here $\underline{A}_N(\mu) \in \mathbb{R}^{N\times N}$ is the SPD matrix with entries $A_{N\,i,j}(\mu) \equiv a(\zeta_j, \zeta_i; \mu)$, $1 \le i, j \le N$, and $\underline{F}_N \in \mathbb{R}^N$ is the "load" (and "output") vector with entries $F_{N\,i} \equiv f(\zeta_i)$, $i = 1, \ldots, N$.

We now invoke (2) to write

$$A_{N\,i,j}(\mu) = a(\zeta_j, \zeta_i; \mu) = \sum_{q=1}^{Q} \sigma^q(\mu)\, a^q(\zeta_j, \zeta_i)\ , \qquad (14)$$

or

$$\underline{A}_N(\mu) = \sum_{q=1}^{Q} \sigma^q(\mu)\, \underline{A}_N^q\ ,$$

where $A^q_{N\,i,j} = a^q(\zeta_j, \zeta_i)$, $i \le i, j \le N$, $1 \le q \le Q$. The off–line/on–line decomposition is now clear. In the *off–line* stage, we compute the $u(\mu_n)$ and form the $\underline{A}_N^q$ and $\underline{F}_N$: this requires N (expensive) "a" finite element solutions and $O(QN^2)$ finite-element-vector inner products. In the *on–line* stage, for any given new μ, we first form $\underline{A}_N$ from (14), then solve (13) for $\underline{u}_N(\mu)$, and finally evaluate $s_N(\mu) = \underline{F}_N^T \underline{u}_N(\mu)$: this requires $O(QN^2) + O(\frac{2}{3}N^3)$ operations and $O(QN^2)$ storage.

Thus, as required, the incremental, or marginal, cost to evaluate $s_N(\mu)$ for any given new μ — as proposed in a design, optimization, or inverse-problem context — is very small: first, because N is very small, typically $O(10)$ — thanks to the good convergence properties of W_N; and second, because (13) can be very rapidly assembled and inverted — thanks to the affine parameter dependence and associated off–line/on–line computational decomposition (see [14] for an earlier application of this strategy within the reduced–basis context). For the problems discussed in this paper, the resulting computational savings relative to standard (well-designed) finite-element approaches are significant — at least $O(10)$, typically $O(100)$, and often $O(1000)$ or more.

IV. A Posteriori Error Estimation: Output Bounds

From Section III we know that, in theory, we can obtain $s_N(\mu)$ very inexpensively: the on–line stage scales as $O(N^3) + O(QN^2)$; and N can, *in theory*, be chosen quite small. However, *in practice*, we do not know *how* small N can be chosen: this will depend on the desired accuracy, the selected output(s) of interest, and the particular problem in question; in some cases $N = 5$ may suffice, while in other cases, $N = 100$ may still be insufficient. In the face of this uncertainty, either too many or too few basis functions will be retained: the former results in computational inefficiency; the latter in unacceptable uncertainty — particularly egregious in the decision contexts in which reduced–basis methods typically serve. We thus need *a posteriori* error estimators for s_N. Surprisingly, *a posteriori* error estimation has received relatively little attention within the reduced–basis framework [8], even though reduced–basis methods are particularly in need of accuracy assessment: the spaces are *ad hoc* and pre-asymptotic, thus admitting relatively little intuition, "rules of thumb," or standard approximation notions.

The approach described here is a particular instance of a general "variational" framework for *a posteriori* error estimation of outputs of interest. However, the reduced–basis instantiation differs significantly from earlier applications to finite element discretization error [25], [26] and iterative solution error [27] both in the choice of (energy) relaxation and in the associated computational artifice. For an alternative approach to reduced–basis error estimates, see [18], [20].

A. Formulation

We assume that we are given a function $g(\mu) : \mathcal{D} \to \mathbb{R}_+$, and a continuous, coercive, symmetric (μ-independent) bilinear form $\hat{a} : X \times X \to \mathbb{R}$ such that

$$\underline{\alpha}_0 \|v\|_X^2 \;\le\; g(\mu)\; \hat{a}(v,v) \;\le\; a(v,v;\mu), \qquad (15)$$

$\forall\; v \in X, \forall\; \mu \in \mathcal{D}$. We then find $\hat{e}(\mu) \in X$ from the modified error equation

$$g(\mu)\; \hat{a}(\hat{e}(\mu), v) \;=\; R(v; u_N(\mu); \mu), \quad \forall v \in X, \qquad (16)$$

where for a given $w \in X$, $R(v;w;\mu) = f(v) - a(w,v;\mu)$ is the weak form of the residual. Our lower and upper output estimators are then evaluated as

$$s_N^-(\mu) \;\equiv\; s_N(\mu), \text{ and } s_N^+(\mu) \;\equiv\; s_N(\mu) + \Delta_N(\mu), \quad (17)$$

respectively, where

$$\Delta_N(\mu) \;\equiv\; g(\mu)\; \hat{a}(\hat{e}(\mu), \hat{e}(\mu)) \qquad (18)$$

is the estimator gap.

B. Properties

We shall prove in this section that $s_N^-(\mu) \le s(\mu) \le s_N^+(\mu)$, and hence that $|s(\mu) - s_N(\mu)| = s(\mu) - s_N(\mu) \le \Delta_N(\mu)$. Our lower and upper output estimators are thus lower and upper output *bounds*; and our output estimator gap is thus an output *bound* gap — a rigorous bound for the error in the output of interest. It is also critical that $\Delta_N(\mu)$ be a relatively *sharp* bound for the true error: a poor (overly large) bound will encourage us to refine an approximation which is, in fact, already adequate — with a corresponding (unnecessary) increase in off–line and on–line computational effort. We shall prove in this section that $\Delta_N(\mu) \le \frac{\gamma_0}{\underline{\alpha}_0}(s(\mu) - s_N(\mu))$, where γ_0 and $\underline{\alpha}_0$ are the *N-independent* a-continuity and $\hat{a}$-coercivity constants defined earlier. Our two results of this section can thus be summarized as

$$1 \;\le\; \eta_N(\mu) \;\le\; \frac{\gamma_0}{\underline{\alpha}_0}, \quad \forall\; N, \qquad (19)$$

where

$$\eta_N(\mu) \;=\; \frac{\Delta_N(\mu)}{s(\mu) - s_N(\mu)}, \qquad (20)$$

is the *effectivity*. We shall denote the left (bounding property) and right (sharpness property) inequalities (19) as the lower effectivity and upper effectivity inequalities respectively.

We now prove the lower effectivity inequality (bounding property): $s_N^-(\mu) \le s(\mu) \le s_N^+(\mu)$, $\forall \mu \in \mathcal{D}$, for $s_N^-(\mu)$ and $s_N^+(\mu)$ defined in (17). The lower bound property directly follows from Section III.B. To prove the upper bound property, we first observe that $R(v;u_N;\mu) = a(u(\mu) - u_N(\mu), v;\mu) = a(e(\mu), v;\mu)$, where $e(\mu) \equiv u(\mu) - u_N(\mu)$; we may thus rewrite (16) as $g(\mu)\hat{a}(\hat{e}(\mu), v) = a(e(\mu), v;\mu)$, $\forall\; v \in X$. We thus obtain

$$\begin{aligned} g(\mu)\hat{a}(\hat{e},\hat{e}) &= g(\mu)\hat{a}(\hat{e}-e, \hat{e}-e) + 2g(\mu)\hat{a}(\hat{e}, e) \\ &\quad - g(\mu)\hat{a}(e,e) \\ &= g(\mu)\hat{a}(\hat{e}-e, \hat{e}-e) + (a(e,e;\mu) \qquad (21) \\ &\quad - g(\mu)\hat{a}(e,e)) + a(e,e;\mu) \\ &\ge a(e,e;\mu) \end{aligned}$$

since $g(\mu)\;\; \hat{a}(\hat{e}(\mu) - e(\mu), \hat{e}(\mu) - e(\mu)) \;\ge\; 0$ and $a(e(\mu), e(\mu);\mu) - g(\mu)\; \hat{a}(e(\mu), e(\mu)) \ge 0$ from (15). Invoking (8) and (21), we then obtain $s(\mu) - s_N(\mu) = a(e(\mu), e(\mu);\mu) \le g(\mu)\; \hat{a}(\hat{e}(\mu), \hat{e}(\mu))$; and thus $s(\mu) \le s_N(\mu) + g(\mu)\; \hat{a}(\hat{e}(\mu), \hat{e}(\mu)) \equiv s_N^+(\mu)$, as desired.

We now prove our second result, the upper effectivity inequality (sharpness property):

$$\eta_N(\mu) = \frac{\Delta_N(\mu)}{s(\mu) - s_N(\mu)} \le \frac{\gamma_0}{\underline{\alpha}_0}, \quad \forall\; N.$$

To begin, we appeal to a-continuity and $\hat{a}$-coercivity to obtain

$$a(\hat{e}(\mu), \hat{e}(\mu);\mu) \;\le\; \frac{\gamma_0\; g(\mu)}{\underline{\alpha}_0} \hat{a}(\hat{e}(\mu), \hat{e}(\mu)). \qquad (22)$$

But from the modified error equation (16) we know that $g(\mu)\hat{a}(\hat{e}(\mu), \hat{e}(\mu)) = R(\hat{e}(\mu);\mu) = a(e(\mu), \hat{e}(\mu);\mu)$. Invoking the Cauchy-Schwartz inequality, we obtain

$$\begin{aligned} g(\mu)\hat{a}(\hat{e},\hat{e}) &= a(e,\hat{e};\mu) \\ &\le (a(\hat{e},\hat{e};\mu))^{1/2}(a(e,e;\mu))^{1/2} \\ &\le \left(\frac{\gamma_0}{\underline{\alpha}_0}\right)^{1/2} (g(\mu)\; \hat{a}(\hat{e},\hat{e}))^{1/2}\; (a(e,e;\mu))^{1/2}; \end{aligned}$$

the desired result then directly follows from (18) and (8).

We now provide empirical evidence for (19). In particular, we present in Table I the bound gap and effectivities for the thermal fin example. Clearly, $\eta_N(\mu)$ is always greater than unity for any N, and bounded — indeed, quite close to unity — as $N \to \infty$.

C. Computational Procedure

Finally, we turn to the computational artifice by which we can efficiently compute $\Delta_N(\mu)$ in the on–line stage of our procedure. We again exploit the affine parameter dependence, but now in a less transparent fashion. To begin, we rewrite the modified error equation, (16), as

$$\hat{a}(\hat{e}(\mu), v) \;=\; \frac{1}{g(\mu)} \left(\ell(v) - \sum_{q=1}^{Q} \sum_{j=1}^{N} \sigma^q(\mu) u_{N\,j}(\mu) a^q(\zeta_j, v) \right),$$

$\forall\; v \in X$, where we have appealed to our reduced–basis approximation (12) and the affine decomposition (2). It

is immediately clear from linear superposition that we can express $\hat{e}(\mu)$ as

$$\hat{e}(\mu) = \frac{1}{g(\mu)} \left(\hat{z}_0 + \sum_{q=1}^{Q} \sum_{j=1}^{N} \sigma^q(\mu) u_{N\,j}(\mu) \hat{z}_j^q \right), \qquad (23)$$

where $\hat{z}_0 \in X$ satisfies $\hat{a}(\hat{z}_0, v) = \ell(v)$, $\forall\ v \in X$, and $\hat{z}_j^q \in X, j = 1, \ldots, N$, $q = 1, \ldots, Q$, satisfies $\hat{a}(\hat{z}_j^q, v) = -a^q(\zeta_j, v)$, $\forall\ v \in X$. Inserting (23) into our expression for the upper bound, $s_N^+(\mu) = s_N(\mu) + g(\mu)\hat{a}(\hat{e}(\mu), \hat{e}(\mu))$, we obtain

$$s_N^+(\mu) = s_N(\mu) + \frac{1}{g(\mu)} \left(c_0 + 2 \sum_{q=1}^{Q} \sum_{j=1}^{N} \sigma^q(\mu) u_{N\,j}(\mu) \Lambda_j^q + \sum_{q=1}^{Q} \sum_{q'=1}^{Q} \sum_{j=1}^{N} \sum_{j'=1}^{N} \sigma^q(\mu) \sigma^{q'}(\mu) u_{N\,j}(\mu) u_{N\,j'}(\mu) \Gamma_{jj'}^{qq'} \right) \qquad (24)$$

where $c_0 = \hat{a}(\hat{z}_0, \hat{z}_0)$, $\Lambda_j^q = \hat{a}(\hat{z}_0, \hat{z}_j^q)$, and $\Gamma_{jj'}^{qq'} = \hat{a}(\hat{z}_j^q, \hat{z}_{j'}^{q'})$. The off–line/on–line decomposition should now be clear.

In the *off–line* stage we compute $\hat{z}_0$ and $\hat{z}_j^q$, $j = 1, \ldots, N$, $q = 1, \ldots, Q$, and then form c_0, Λ_j^q, and $\Gamma_{jj'}^{qq'}$: this requires $QN+1$ (expensive) "$\hat{a}$" finite element solutions, and $O(Q^2N^2)$ finite-element-vector inner products. In the *on–line* stage, for any given new μ, we evaluate s_N^+ as expressed in (24): this requires $O(Q^2N^2)$ operations; and $O(Q^2N^2)$ storage (for c_0, Λ_j^q, and $\Gamma_{jj'}^{qq'}$). As for the computation of $s_N(\mu)$, the marginal cost for the computation of $s_N^+(\mu)$ for any given new μ is quite small — in particular, it is *independent* of the dimension of the truth finite element approximation space X.

There are a variety of ways in which the off–line/on–line decomposition and output error bounds can be exploited. A particularly attractive mode incorporates the error bounds into an on–line adaptive process, in which we successively approximate $s_N(\mu)$ on a sequence of approximation spaces $W_{N_j'} \subset W_N, N_j' = N_0 2^j$ — for example, $W_{N_j'}$ may contain the N_j' sample points of S_N closest to the new μ of interest — until $\Delta_{N_j'}$ is less than a specified error tolerance. This procedure both minimizes the on–line computational effort and reduces conditioning problems — while simultaneously ensuring both accuracy and certainty.

Acknowledgments

We would like to thank Mr. Thomas Leurent (formerly) of MIT for his many contributions to the work described in this paper; thanks also to Shidati Ali of the Singapore-MIT Alliance and Yuri Solodukhov for very helpful discussions. We would also like to acknowledge our longstanding collaborations with Professor Jaime Peraire of MIT and Professor Einar Røquist of the Norwegian University of Science and Technology. This work was supported by the Singapore-MIT Alliance, by DARPA and ONR under Grant F49620-01-1-0458, by DARPA and AFOSR under Grant N00014-01-1-0523 (Subcontract 340-6218-3) and by NASA under Grant NAG-1-1978.

References

[1] T.F. Chan and W.L. Wan, "Analysis of projection methods for solving linear systems with multiple right-hand sides," *SIAM Journal on Scientific Computing*, vol. 18, no. 6, pp. 1698, 1721 1997.

[2] C. Farhat, L. Crivelli, and F.X. Roux, "Extending substructure based iterative solvers to multiple load and repeated analyses," *Computer Methods in Applied Mechanics and Engineering*, vol. 117, no. 1-2, pp. 195–209, July 1994.

[3] M.A. Akgun, J.H. Garcelon, and R.T. Hartka, "Fast exact linear and non-linear structural reanalysis and the Sherman-Morrison-Woodbury formulas," *International Journal for Numerical Methods in Engineering*, vol. 50, no. 7, pp. 1587–1606, March 2001.

[4] E.L. Yip, "A note on the stability of solving a rank-p modification of a linear system by the Sherman-Morrison-Woodbury formula," *SIAM Journal on Scientific and Statistical Computating*, vol. 7, no. 2, pp. 507–513, April 1986.

[5] E. Allgower and K. Georg, "Simplicial and continuation methods for approximating fixed-points and solutions to systems of equations," *SIAM Review*, vol. 22, no. 1, pp. 28–85, 1980.

[6] W.C. Rheinboldt, "Numerical analysis of continuation methods for nonlinear structural problems," *Computers and Structures*, vol. 13, no. 1-3, pp. 103–113, 1981.

[7] B. O. Almroth, P. Stern, and F. A. Brogan, "Automatic choice of global shape functions in structural analysis," *AIAA Journal*, vol. 16, pp. 525–528, May 1978.

[8] A. K. Noor and J. M. Peters, "Reduced basis technique for nonlinear analysis of structures," *AIAA Journal*, vol. 18, no. 4, pp. 455–462, April 1980.

[9] A. Barrett and G. Reddien, "On the reduced basis method," *Math. Mech.*, vol. 7, no. 75, pp. 543–549, 1995.

[10] J. P. Fink and W. C. Rheinboldt, "On the error behaviour of the reduced basis technique for nonlinear finite element approximations," *Z. Angew. Math. Mech.*, vol. 63, pp. 21–28, 1983.

[11] J. S. Peterson, "The reduced basis method for incompressible viscous flow calculations," *SIAM J. Sci. Stat. Comput.*, vol. 10, no. 4, pp. 777–786, July 1989.

[12] T. A. Porsching, "Estimation of the error in the reduced basis method solution of nonlinear equations," *Mathematics of Computation*, vol. 45, no. 172, pp. 487–496, October 1985.

[13] W.C. Rheinboldt, "On the theory and error estimation of the reduced basis method for multi-parameter problems," *Nonlinear Analysis, Theory, Methods and Applications*, vol. 21, no. 11, pp. 849–858, 1993.

[14] E. Balmes, "Parametric families of reduced finite element models. theory and applications," *Mechanical Systems and Signal Processing*, vol. 10, no. 4, pp. 381–394, 1996.

[15] L. Machiels, Y. Maday, I. B. Oliveira, A.T. Patera, and D.V. Rovas, "Output bounds for reduced-basis approximations of symmetric positive definite eigenvalue problems," *C. R. Acad. Sci. Paris, Série I*, vol. 331, no. 2, pp. 153–158, July 2000.

[16] Y. Maday, L. Machiels, A. T. Patera, and D. V. Rovas, "Blackbox reduced-basis output bound methods for shape optimization," in *Proceedings 12^{th} International Domain Decomposition Conference*, Japan, 2000, to appear.

[17] Y. Maday, A.T. Patera, and D.V. Rovas, "A blackbox reduced-basis output bound method for noncoercive linear problems," *Nonlinear Partial Differential Equations and Their Applications*, 2001, College De France Seminar. To appear.

[18] C. Prud'homme, D. Rovas, K. Veroy, Y. Maday, A.T. Patera, and G. Turinici, "Reliable real-time solution of parametrized partial differential equations: Reduced-basis output bounds methods," *Journal of Fluids Engineering*, 2002, to appear.

[19] L. Machiels, A.T. Patera, and D.V. Rovas, "Reduced basis output bound methods for parabolic problems," *in progress*, 2001.

[20] K. Veroy, T. Leurent, C. Prud'homme, D. Rovas, and A.T. Patera, "Reliable real–time solution of parametrized elliptic partial differential equations: Application to elasticity," in *SMA Symposium*, January 2002.

[21] Y. Solodukhov, Ph.D. thesis, Massachusetts Institute of Technology, 2004, in progress.

[22] D. Rovas, *Reduced-Basis Output Bound Methods for Partial Differential Equations*, Ph.D. thesis, Massachusetts Institute of Technology, 2002, in progress.

[23] Y. Maday, A.T. Patera, and G. Turinici, "A priori convergence theory for approximation of simple–parameter elliptic partial dif-

ferential equations," *C. R. Acad. Sci. Paris, Série I*, 2001, submitted.

[24] K. Veroy, *Reduced Basis Methods Applied to Problems in Elasticity: Analysis and Applications*, Ph.D. thesis, Massachusetts Institute of Technology, 2003, in progress.

[25] Y. Maday, A. T. Patera, and J. Peraire, "A general formulation for a posteriori bounds for output functionals of partial differential equations; Application to the eigenvalue problem," *C. R. Acad. Sci. Paris, Série I*, vol. 328, pp. 823–828, 1999.

[26] L. Machiels, J. Peraire, and A. T. Patera, "A posteriori finite element output bounds for the incompressible Navier-Stokes equations; Application to a natural convection problem," *Journal of Computational Physics*, pp. 401–425, 2000.

[27] A. T. Patera and E. M. Rønquist, "A general output bound result: Application to discretization and iteration error estimation and control," *Math. Models Methods Appl. Sci.*, vol. 11(4), pp. 685–712, 2001.